3. CHEMICAL AND PHYSICAL INFORMATION

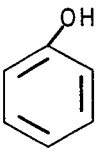
3.1 CHEMICAL IDENTITY

Information regarding the chemical identity of phenol is located in Table 3-l.

3.2 PHYSICAL AND CHEMICAL PROPERTIES

Information regarding the physical and chemical properties of phenol is located in Table 3-2.

TABLE 3-1. Chemical Identity of Phenol

Characteristic	Information	Reference
Chemical name	Phenol	Lide 1993
Synonym(s)	Benzenol, hydroxybenzene, monophenol, oxybenzene, phenyl alcohol, phenyl hydrate, phenyl hydroxide, phenylic acid, phenylic alcohol	Lewis 1996
Registered trade name(s)	Carbolic acid, phenic acid, phenic alcohol	Gardner et al. 1978
Chemical formula	C_6H_6O	Lide 1993
Chemical structure		Budavari et al. 1989
Identification numbers:		
CAS registry	108-95-2	OHM/TADS 1998
NIOSH RTECS	SJ3325000	RTECS 1998
EPA hazardous waste	U188	EPA 1998b
OHM/TADS	7216849	OHM/TADS 1998
DOT/UN/NA/IMO shipping	IMO 6.1 UN 1671 (solid) UN 2312 (molten) UN 2821 (solution)	HSDB 1997
HSDB	113	HSDB 1998
NCI	C50124	Lewis 1996

CAS = Chemical Abstracts Services; DOT/UN/NA/IMO = Department of Transportation/United Nations/North America/International Maritime Dangerous Goods Code; EPA = Environmental Protection Agency; HSDB = Hazardous Substances Data Bank; NCI = National Cancer Institute; NIOSH = National Institute for Occupational Safety and Health; OHM/TADS = Oil and Hazardous Materials/ Technical Assistance Data System; RTECS = Registry of Toxic Effects of Chemical Substances

TABLE 3-2. Physical and Chemical Identity of Phenol

Property	Information	Reference
Molecular weight	94.11	Lide 1993
Color	Colorless to light pink	HSDB 1998
Physical state	Crystalline solid liquid (w/8% H_2O)	
Melting point	43°C	Lide 1993
Boiling point	181.8°C	Lide 1993
Density:		
At 20°C	1.0545@45°C/4°C	Lide 1993
Vapor density	3.24	Lewis 1996
Odor	Distinct aromatic, somewhat sickening, sweet and acrid odor	HSDB 1998
Odor threshold:		
Water	7.9 ppm (w/v)	Amoore and Hautala 1983
	1 ppm (w/v)	Baker et al. 1978
Air	0.040 ppm (v/v)	Amoore and Hautala 1983
Solubility:		
Water at 25°C	87 g/L	Lide 1993
Organic solvent(s)	Very soluble in alcohol, chloroform, ether, benzine, acetone, water	Lide 1993
Partition coefficients:		
Log K_{ow}	1.46	HSDB 1998
Log K_{oc}	1.21–1.96	Artiola-Fortuny and Fuller 1982; Boyd 1982; Briggs 1981; Sacan and Balcioglu 1996; Scott et al. 1983
Vapor pressure:		
at 25°C	0.3513	HSDB 1998
Henry's law constant:	4.0×10^{-7} m^3/mol	Lide 1993
Autoignition temperature	715°C	Lewis 1996
Flashpoint, open cup	85°C	HSDB 1998
Flashpoint, closed cup	79°C	NIOSH 1997
Flammability limits (in air, by % v)	1.7%–8.6%	NIOSH 1997
Conversion factors:		
ppm (v/v) to mg/m^3 in air (20°C)	ppm (v/v) × 3.92 = mg/m^3	
mg/m^3 to ppm (v/v) in air (20°C)	mg/m^3 × 0.255 = ppm (v/v)	

atm = atmosphere; v = volume; w = weight